STEADY STATES OF THE 1D DOI-ONSAGER MODEL IN THE STRONG SHEAR FLOW[*]

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Abstract. Here we will investigate the steady states of the Doi-Onsager model in general shear flows. Generally we know that the equilibrium is not the Maxwell-Boltzmann distribution in the shear flow. Here we will give not only the expression of the equilibrium for the 1D Doi-Onsager model in shear flows by rigorous proof, but also a discussion of the critical points of the intensity α and the shear rate γ by numerical calculation. The equilibrium of the particles depends on the competition between the parameters α and γ. When α crosses the first critical point $\alpha_1 \approx 4.083$ from a smaller value, the number of steady states will change from one to three through two. At the same time the shear rate γ depends on α. When α crosses the second critical point $\alpha_2 \approx 5.125$ from smaller values, the number of steady states will change from three to one through two for some related γ. It can be found that some of the equilibria are stable with respect to the energy functional. These results are partly consistent with the work of Marrucci and Maffettone in [20], in which formal analysis was given.

Key words. Steady states, strong shear flow, Doi-Onsager model, critical points.

AMS subject classifications. 82B27, 35Q35.

1. Introduction

It is well-known that the Doi model can describe the dynamical states in dilute polymeric fluids. We consider the behaviour of chain molecules or rod particles. Important effects were found in some numerical simulations, e.g., [9, 10, 11, 14, 19, 20], and theoretical analysis, e.g., [1, 2, 3, 26]. In the simplest case of no flow (velocity $u = 0$), it is also called Doi-Onsager model [17, 23, 25]. It can describe phase transition phenomena though it is very simple. Therefore, this model has recently attracted considerable attention [4, 5, 6, 14], especially in the mathematics community [1, 2, 3, 7, 8, 12, 13, 16, 17, 18, 23, 24]. At first, Onsager [22] showed in 1949 that the steady state is the prolate phase when the intensity among the particles is strong. The prolate phase consists of aligned particles. He derived this result via a variational approach under the assumption that the equilibrium was axially symmetric and possessed some explicit expression for the Onsager interaction potential between molecules. This name was attributed to the potential by later authors. In 1959 Maier and Saupe [21] investigated the nematic phase for a simpler potential among the molecules, which is now called Maier-Saupe potential, e.g., [4, 5]. In 2005, a rigorous proof of the Onsager assumption for the Maier-Saupe potential was given in [17, 8, 23]. Meanwhile explicit expressions for all equilibria were shown in [3, 17]. The phase transition phenomenon was proved in the investigation of stability of these equilibria [24]. In [24], many steady states were found in the weak flow for the Doi model, such as flow-aligning, tumbling, log-rolling, and kayaking. Concerning the asymptotic states and the properties of the Doi-Onsager model without flow, Constantin et al. [1, 2] gave many very interesting

results. Here we will investigate the equilibrium of the Doi-Onsager model in the strong shear flow while we restrict ourselves to rodlike particles on the circle.

The mathematical model we adopt is the Doi-Onsager equation on the circle for shear flow

$$\psi_t = D_r[\psi_{\theta\theta} + (\psi U_\theta)_\theta] + \gamma(\psi\sin^2\theta)_\theta, \tag{1.1}$$

where $\psi(\theta,t)$ denotes the orientational probability distribution function (PDF) for rod-like, rigid molecules. The constant D_r is the averaged rotational diffusivity, which will be set to 1. The parameter γ is the shear rate. The function U is the mean-field interaction potential, which here is considered to be the Maier-Saupe potential [21] given as

$$U = \alpha \int_0^{2\pi} \sin^2(\theta - \theta')\psi(\theta',t)d\theta'. \tag{1.2}$$

The parameter α describes the interaction intensity among the rod particles. Furthermore, we know that $\psi(\theta,t)$ is 2π periodic in θ. We are seeking solutions that satisfy $\psi \geq 0$ and the normalization condition

$$\int_0^{2\pi} \psi(\theta,t)d\theta = 1. \tag{1.3}$$

When there is no flow, all equilibria of equation (1.1) were given in [3, 16]. It was shown that if the interaction intensity parameter α is less than 4, the constant solution is the only possible steady state solution, which describes the isotropic phase. If α is larger than 4, then there is a new solution that corresponds to the nematic phase. All other non-constant solutions are obtained from this solution by translation. It was also proved that the nematic solutions have period π instead of 2π, which signifies the fact that the rods are symmetric, i.e., they have orientations but no directions. Later in [17], a new simple approach to reprove these results was found. Moreover, an explicit expression for all the solutions was given in [17], which is

THEOREM 1.1. [17] The number of stationary solutions to (1.1)–(1.3) with $\gamma = 0$ depends on whether the intensity crosses the critical value $\alpha = 4$. More precisely,

(i) If $\alpha \leq 4$, then the only stationary solution is the constant $f = 1/2\pi$.

(ii) If $\alpha > 4$, then besides the constant solution $f = 1/2\pi$, all other stationary solutions are given by

$$f(\theta) = \frac{1}{\tilde{Z}} e^{-\eta^* \cos 2(\theta - \theta_0)}, \tag{1.4}$$

where $\tilde{Z} = \int_0^{2\pi} e^{-\eta^* \cos 2\theta}d\theta$ and θ_0 is arbitrary. $\eta^* > \frac{\alpha}{2}\sqrt{1 - 4/\alpha}$ is uniquely determined by the equation

$$\frac{\int_0^{2\pi} \cos 2\theta \ e^{-\eta^* \cos 2\theta}d\theta}{\int_0^{2\pi} e^{-\eta^* \cos 2\theta}d\theta} + \frac{2\eta^*}{\alpha} = 0. \tag{1.5}$$

There are complete theoretical results for the full Doi model on a sphere given in [17]. All equilibrium solutions are necessarily uniaxially symmetric, see [17, 23, 8]. The number of equilibrium states and their qualitative behavior for the Doi-Onsager

equation hinge on whether the intensity α crosses two critical values [17]. It is also shown that there is a phase transition when α changes. Additionally, we can see the hysteresis phenomenon when the intensity α changes from small to large and from large to small in [24].

In this paper we will determine all equilibria of the Doi equation on the circle under strong shear flows. We obtain the result that there is no isotropic phase and all equilibria are in the nematic phase.

THEOREM 1.2. *The PDF ψ of the equilibria of* (1.1)–(1.3) *possesses the form*

$$\psi(\theta) = \frac{1}{Z}[1+b(\theta)]e^{-a(\theta)}, \tag{1.6}$$

where

$$a(\theta) = \frac{\alpha}{2} + \eta\cos 2(\theta-\theta_0) + \frac{\gamma\theta}{2}, \tag{1.7}$$

$$b(\theta) = (e^{\gamma\pi}-1)\frac{\int_0^\theta e^{a(\tau)}d\tau}{\int_0^{2\pi} e^{a(\tau)}d\tau}, \tag{1.8}$$

and Z is the normalization constant, given by

$$Z = \int_0^{2\pi}[1+b(\theta)]e^{-a(\theta)}d\theta. \tag{1.9}$$

Furthermore, the parameters η and θ_0 are determined by the intensity α and the shear rate γ through the relations

$$\frac{\int_0^{2\pi}\cos 2(\theta-\theta_0)[1+b(\theta)]\ e^{-a(\theta)}d\theta}{\int_0^{2\pi}[1+b(\theta)]\ e^{-a(\theta)}d\theta} + \frac{2\eta}{\alpha} + \frac{\gamma}{2\alpha}\sin 2\theta_0 = 0, \tag{1.10}$$

$$\frac{\int_0^{2\pi}\sin 2(\theta-\theta_0)[1+b(\theta)]\ e^{-a(\theta)}d\theta}{\int_0^{2\pi}[1+b(\theta)]\ e^{-a(\theta)}d\theta} + \frac{\gamma}{2\alpha}\cos 2\theta_0 = 0. \tag{1.11}$$

Comparing the expression (1.6) with (1.4), we can formally see how far the equilibrium of the 1D Doi model in the general shear flow is from the Boltzmann distribution (1.4) without shear flow. Let us change the form of (1.6) slightly as follows:

$$\psi(\theta) = \frac{\tilde{Z}}{Z_1}e^{-\frac{\gamma\theta}{2}}\frac{1}{\tilde{Z}}e^{-\eta\cos 2(\theta-\theta_0)} + \frac{1}{Z}b(\theta)e^{-a(\theta)},$$

where $Z_1 = \int_0^{2\pi}e^{-(\frac{\gamma\theta}{2}+\eta\cos 2(\theta-\theta_0))}d\theta$ and we have deleted a term $e^{-\alpha/2}$. Here the first term is a dilation of $\frac{\tilde{Z}}{Z_1}e^{-\frac{\gamma\theta}{2}}$ of the Boltzmann distribution (1.4) due to the shear flow, and we can take the second term as the additional perturbation of the Boltzmann distribution (1.4).

Unfortunately, here we cannot theoretically analyze equations (1.10) and (1.11) to find the critical points of the intensity parameter α and the shear rate γ. However, by numerical calculations for (1.10) and (1.11), it can be shown that the critical points of the intensity α and the shear rate γ are approximate. Precisely, we find the following results:

(a) When $0 < \alpha < \alpha_1(\alpha_1 \approx 4.083)$, there is only one pair of (η, θ_0) to satisfy (1.10) and (1.11). This implies that the equilibrium is uniquely determined by the intensity

α and the shear rate γ when α is less than the first critical point α_1 and γ is any given positive constant. Moreover, for $\alpha \in]0, \alpha_1[$ fixed, the solution (η, θ_0) depends on the shear rate γ and θ_0 is not a monotone function of γ. There is a critical point for γ such that θ_0 attains a minimum; for example, $\gamma = 3.5$ is the critical point for $\alpha = 1.0$ (figure 2.7). We can see that η is a monotone increasing function of γ for fixed α from Tables 2.1, 2.2 and 2.3 .

(b) When $\alpha_1 < \alpha < \alpha_2 (\alpha_2 \approx 5.125)$, there are possibly many pairs of solutions (η, θ_0) to satisfy (1.10) and (1.11) for some γ. The number of solutions depends on the choice of γ. It shows that the equilibrium of the particles in a polymeric fluid is possible for many steady states, but some steady states are not stable. For example, we can see that $(\eta, \theta_0) = (0.1333, 0.8374), (0.967, 1.728), (1.0596, 1.935)$ are solutions of (1.10) and (1.11) for $\gamma = 0.01$ and $\alpha = 4.5$ from Table 2.2. But the solution $(0.1333, 0.8374)$ is unstable with respect to the energy functional, while for $\alpha = 4.5$ and $\gamma = 0.1685$, there are two stable solutions $(\eta, \theta_0) = (0.6, 1.025), (1.1346, 1.9092)$. But when $\alpha = 4.5$ and $\gamma > 0.6$, there is only one solution. Moreover, it can be found that γ depends on α for which there are multiple steady states.

(c) When $\alpha > \alpha_2$, there is only one solution (η, θ_0) which satisfies (1.10) and (1.11). This implies that the steady state of the molecules in the flow is also uniquely determined by the interaction intensity α and shear rate γ. Moreover, for $\alpha \in]\alpha_2, \infty[$ fixed, θ_0 and η are increasing functions of the shear rate γ, e.g., from (figure 2.10), we can see the profile of $\theta_0(\gamma)$ for $\alpha = 8.0$.

Here we especially point out that these results are partly consistent with the work of Marrucci and Maffettone in [20]. They **formally** analyzed the explicit expression for PDF $\psi = Ce^{-g(\phi)}(\int_0^\phi e^{-g(x)} dx + K)$ with $g(\phi) = -a\cos 2\phi + G(\phi - \frac{1}{2}\sin(2\alpha + 2\phi))$ and $a = U \int_0^\pi \psi(\phi) \cos 2\phi d\phi$ by introducing $\theta = \phi + \beta$, where β is the angular shift $(-\pi/4 \le \beta \le \pi/4)$. The latter is chosen so as to obtain

$$\int_0^\pi \psi(\phi) \sin 2\phi d\phi = 0. \qquad (1.12)$$

In fact, the parameter G is $\frac{1}{2}\gamma$, and U is about $\frac{1}{2}\alpha$ in our paper since we use the different parameters with a different meaning. Then the result about the critical point of α and γ was obtained by numerical calculation to (1.12) for given parameters a and β in [20]. It is stated in [20] that:

the solution is not always found, however. We find one (and only one) solution throughout the range of G values explored ($0 < G < 10^3$) only for values of U less than ca. 2.41, thus encompassing the whole isotropic range ($0 \le U \le 2$), as well as a small segment of the nematic range ($2 < U < 2.41$). Conversely, for $U > 2.41$, a lower bound for G is found, call $G_{critical}$, below which the stationary solution disappears. We infer that, for $G < G_{critical}$, the system switches to the tumbling situation. $G_{critical}$ appears to grow steadily with increasing U.

Their result was partially correct in virtue of the formal solution. Here we rigorously deduce the form of the solution, and we definitely find that the isotropic solution $\psi = \frac{1}{2\pi}$ does not satisfy the steady state equation (2.2). So it is obvious that there is no isotropic phase for any positive values of the parameters α and γ. Furthermore, when α is larger than ca. 5.125, the unique stationary state is the nematic phase for any values of the shear rate γ. This is also consistent with the result for the case of no flow, see [3, 7, 16, 17, 20], which states that the unique stationary state is the nematic phase for $\alpha > 4$. In our result we have not found the tumbling situation, which was

reported in [20], since it is not stable stationary state, . In this work we report that there are two stable stationary states for $\alpha \in]4.083, 5.125[$ and some shear rate γ. It is possibly due to the presence of wagging state for the time dynamic system. The boundary states of the wagging case would be the stable steady states we found.

In addition, there is a paper [15], in which the weak shear case was investigated for the dynamic model (1.1) with a variety of moment closure approaches. The authors obtained the weak-shear solvability conditions for persistence of equilibria due to the shear-perturbed approach, nearly isotropic branch (using bifurcation software that gives full phase diagram whose regions are separated by bifurcations). These phase diagrams and all bifurcations were compared with the work [21]. Here we directly investigate the steady state equation of the model (1.1) without any closure approach. We also claim that there are one or two stable steady states for some intensity parameter α and the shear rate γ, which are consistent with the diagram of mesoscopic models in [15].

This paper is organized as follows. Section 2 is devoted to the analysis of the expression and some properties of the equilibrium states in the general shear flow. Meanwhile, we will discuss the critical points of the intensity parameter α and the shear rate γ, in which the number of the equilibrium changes. In section 3 the stability of multiple solutions was discussed by calculating the energy functional. Then conclusions are drawn in the final section.

2. Steady states in the shear flow

In this section we will explicitly investigate the expression of the steady states of equation (1.1) in the shear flow. It follows from (1.2) that

$$U_\theta = \alpha \int_0^{2\pi} \sin 2(\theta - \theta') \psi(\theta', t) d\theta'.$$

Furthermore,

$$\begin{aligned} U_{\theta\theta} &= 2\alpha \int_0^{2\pi} \cos 2(\theta - \theta') \psi(\theta', t) d\theta' \\ &= 2\alpha \int_0^{2\pi} [1 - 2\sin^2(\theta - \theta')] \psi(\theta', t) d\theta' \\ &= 2\alpha - 4U, \end{aligned}$$

where (1.3) has been used. Therefore, we obtain a decoupled equation for U

$$U_{\theta\theta} + 4U = 2\alpha.$$

Its general solution is

$$U = \frac{\alpha}{2} + s_1 \cos 2\theta + s_2 \sin 2\theta, \tag{2.1}$$

where s_1, s_2 are two parameters.

We consider the steady states, which satisfy

$$0 = \psi_{\theta\theta} + (\psi U_\theta)_\theta + \gamma(\psi \sin^2 \theta)_\theta \tag{2.2}$$

and (2.1). Integration of (2.2) from 0 to θ yields

$$\psi_\theta + \psi U_\theta + \gamma \psi \sin^2 \theta = C, \tag{2.3}$$

where C is a constant that is independent of θ. If the shear rate $\gamma = 0$, we can easily prove that $C \equiv 0$ in the above equation similar to [16, 17]. Thus the distribution is the Boltzmann distribution $\psi = \frac{1}{Z} e^{-U}$, where Z is the normalization. However we have $C \neq 0$ when $\gamma \neq 0$. In the following we want to determine C in (2.3).

Integration of (2.3) from 0 to 2π yields

$$\int_0^{2\pi} \psi_\theta d\theta + \int_0^{2\pi} \psi U_\theta d\theta + \int_0^{2\pi} \gamma \psi \sin^2 \theta d\theta = 2\pi C. \tag{2.4}$$

The first term in (2.4) is *zero* since ψ is a periodic function of period 2π. We denote the second term by G. Then

$$G = \int_0^{2\pi} \psi U_\theta d\theta$$
$$= \alpha \int_0^{2\pi} \int_0^{2\pi} \sin 2(\theta - \theta') \psi(\theta) \psi(\theta') d\theta' d\theta$$
$$= \alpha \int_0^{2\pi} \int_0^{2\pi} (\sin 2\theta \cos 2\theta' - \cos 2\theta \sin 2\theta') \psi(\theta) \psi(\theta') d\theta' d\theta$$
$$= 0.$$

The last equality is easily seen by writing the difference as two separate integrals and interchanging the variables in one of them. So (2.4) implies

$$\int_0^{2\pi} \gamma \psi(\theta) \sin^2 \theta d\theta = 2\pi C.$$

Thus, we can obtain

$$C = \frac{\gamma}{2\pi} \int_0^{2\pi} \sin^2 \theta \psi(\theta) d\theta > 0. \tag{2.5}$$

Now we introduce $a'(\theta) = U_\theta + \gamma \sin^2 \theta$, then

$$a(\theta) = U + \gamma \left(\frac{\theta}{2} - \frac{1}{4} \sin 2\theta \right)$$
$$= \frac{\alpha}{2} + s_1 \cos 2\theta + s_2 \sin 2\theta + \gamma \left(\frac{\theta}{2} - \frac{1}{4} \sin 2\theta \right)$$
$$= \frac{\alpha}{2} + \eta \cos 2(\theta - \theta_0) + \frac{\gamma \theta}{2}, \tag{2.6}$$

where η and θ_0 are two new parameters replacing s_1, s_2 which satisfy

$$\eta^2 = s_1^2 + (s_2 - \gamma/4)^2, \quad \tan 2\theta_0 = (s_2 - \gamma/4)/s_1.$$

Without the loss of the generality we assume here that $\eta > 0$. For $\eta < 0$ we can modify the definition of θ_0 to $\theta_0 + \pi/2$ to give the same form of $a(\theta)$. Then from (2.3), we can obtain

$$(\psi e^{a(\theta)})_\theta = C e^{a(\theta)}. \tag{2.7}$$

Integration of (2.7) from 0 to θ yields

$$\psi(\theta) e^{a(\theta)} = K + C \int_0^\theta e^{a(\tau)} d\tau,$$

where K is a constant. Therefore, we obtain that the distribution function is

$$\psi(\theta) = Ke^{-a(\theta)} + Ce^{-a(\theta)} \int_0^\theta e^{a(\tau)} d\tau, \tag{2.8}$$

where $a(\theta)$ and C are given by (2.6) and (2.5), respectively. Here we can see that there are five parameters $K, \alpha, \gamma, \eta, \theta_0$ in the expression (2.8). However they are not completely independent. They certainly satisfy some relations as follows:

(1) The distribution function $\psi(\theta)$ satisfies the normalization (1.3). So we have

$$K \int_0^{2\pi} e^{-a(\theta)} d\theta + C \int_0^{2\pi} e^{-a(\theta)} \int_0^\theta e^{a(\tau)} d\tau d\theta = 1. \tag{2.9}$$

(2) The function $\psi(\theta)$ is periodic, i.e., $\psi(2\pi) = \psi(0)$. From (2.8) and (2.6), we obtain

$$\psi(2\pi) = Ke^{-a(2\pi)} + Ce^{-a(2\pi)} \int_0^{2\pi} e^{a(\tau)} d\tau, \quad \psi(0) = Ke^{-a(0)},$$

$$a(2\pi) = \frac{\alpha}{2} + \eta \cos 2\theta_0 + \gamma\pi = a(0) + \gamma\pi.$$

Thus, we have from $\psi(2\pi) = \psi(0)$ the relation

$$K[e^{\gamma\pi} - 1] = C \int_0^{2\pi} e^{a(\tau)} d\tau. \tag{2.10}$$

From the relation (2.10) we can see that K has the same sign as the shear rate γ because $C > 0$ and $\int_0^{2\pi} e^{a(\tau)} d\tau > 0$.

(3) On the other hand, from (2.1) and (2.6)

$$U = \frac{\alpha}{2} + s_1 \cos 2\theta + s_2 \sin 2\theta$$

$$= \frac{\alpha}{2} + \eta \cos 2(\theta - \theta_0) + \frac{\gamma}{4} \sin 2\theta. \tag{2.11}$$

Invoking (1.2) we have

$$\frac{\alpha}{2} + \eta \cos 2(\theta - \theta_0) + \frac{\gamma}{4} \sin 2\theta = \alpha \int_0^{2\pi} \sin^2(\theta - \theta') \psi(\theta') d\theta. \tag{2.12}$$

From the above relations (2.9)-(2.12) for the parameters $K, \alpha, \gamma, \eta, \theta_0$, we can now conclude the result of Theorem 1.2.

The proof of Theorem 1.2.

Proof. From (2.10) we obtain

$$C = K \frac{e^{\gamma\pi} - 1}{\int_0^{2\pi} e^{a(\tau)} d\tau}.$$

We insert this into (2.8) to obtain

$$\psi(\theta) = K \left[1 + \frac{e^{\gamma\pi} - 1}{\int_0^{2\pi} e^{a(\tau)} d\tau} \int_0^\theta e^{a(\tau)} d\tau \right] e^{-a(\theta)}.$$

Now the definition $Z = 1/K$, $b(\theta)$ given by (1.8), and $a(\theta)$ already defined in (2.6) gives the form (1.6) of the solution. The formula (1.9) for Z is defined by (2.9) using (2.10) again. Finally we insert the solution (1.6) into (2.12) to obtain

$$\frac{\int_0^{2\pi} \sin^2(\theta - \theta')[1 + b(\theta')] \ e^{-a(\theta')} d\theta'}{Z} = \frac{1}{2} + \frac{\eta}{\alpha} \cos 2(\theta - \theta_0) + \frac{\gamma}{4\alpha} \sin 2\theta. \quad (2.13)$$

Now combining (2.13) with (1.9) for the nonlocal term Z we can obtain

$$\frac{\int_0^{2\pi} \sin^2(\theta - \theta')[1 + b(\theta')] \ e^{-a(\theta')} d\theta'}{\int_0^{2\pi}[1 + b(\theta)] \ e^{-a(\theta)} d\theta} = \frac{1}{2} + \frac{\eta}{\alpha} \cos 2(\theta - \theta_0) + \frac{\gamma}{4\alpha} \sin 2\theta$$

$$= \frac{1}{2} + [\frac{\eta}{\alpha} + \frac{\gamma}{4\alpha} \sin 2\theta_0] \cos 2(\theta - \theta_0) + \frac{\gamma}{4\alpha} \cos 2\theta_0 \sin 2(\theta - \theta_0). \quad (2.14)$$

Since

$$\sin^2(\theta - \theta') = \frac{1}{2}[1 - \cos 2(\theta - \theta')] = \frac{1}{2} - \frac{1}{2} \cos[2(\theta - \theta_0) + 2(\theta_0 - \theta')]$$

$$= \frac{1}{2} - \frac{1}{2}[\cos 2(\theta - \theta_0) \cos 2(\theta_0 - \theta') - \sin 2(\theta - \theta_0) \sin 2(\theta_0 - \theta')]$$

$$= \frac{1}{2} - \frac{1}{2}[\cos 2(\theta - \theta_0) \cos 2(\theta' - \theta_0) + \sin 2(\theta - \theta_0) \sin 2(\theta' - \theta_0)],$$

we have that the left side of (2.14) is equal to

$$\frac{1}{2} - \frac{1}{2} \frac{\int_0^{2\pi} \cos 2(\theta' - \theta_0)[1 + b(\theta')] \ e^{-a(\theta')} d\theta'}{\int_0^{2\pi}[1 + b(\theta)] \ e^{-a(\theta)} d\theta} \cos 2(\theta - \theta_0)$$

$$- \frac{1}{2} \frac{\int_0^{2\pi} \sin 2(\theta' - \theta_0)[1 + b(\theta')] \ e^{-a(\theta')} d\theta'}{\int_0^{2\pi}[1 + b(\theta)] \ e^{-a(\theta)} d\theta} \sin 2(\theta - \theta_0).$$

Using the linear independence of $\cos 2(\theta - \theta_0)$ and $\sin 2(\theta - \theta_0)$ gives the two relations (1.10) and (1.11).   □

From the expression (1.6) we can see that the distribution function ψ is an approximate Boltzmann distribution (1.4) in [17] when the shear rate γ is sufficiently small since

$$e^{\gamma \pi} - 1 \approx 0 \text{ as } \gamma \ll 1$$

and

$$\frac{\alpha}{2} + \eta \cos 2(\theta - \theta_0) + \frac{\gamma \theta}{2} \approx \frac{\alpha}{2} + \eta \cos 2(\theta - \theta_0) \text{ as } \gamma \ll 1.$$

Next we will prove the periodicity property of this distribution function in the strong shear flow similar to the equilibrium of the distribution function in no flow [16, 17].

PROPOSITION 2.1. *The solution $\psi(\theta)$ defined by (1.6) is periodic with period π.*

Proof. By using (1.7), we can obtain

$$\int_0^{\theta + \pi} e^{a(\tau)} d\tau = (\int_0^{\pi} + \int_{\pi}^{\theta + \pi}) e^{a(\tau)} d\tau$$

$$= \int_0^{\pi} e^{a(\tau)} d\tau + e^{\frac{\gamma \pi}{2}} \int_0^{\theta} e^{a(\tau)} d\tau.$$

Thus, in virtue of (1.6)–(1.8)

$$\psi(\theta+\pi) = \frac{1}{Z}[1+b(\theta+\pi)]e^{-a(\theta+\pi)}$$

$$= \frac{1}{Z}\left[1+\frac{e^{\gamma\pi}-1}{\int_0^{2\pi}e^{a(\tau)}d\tau}\left(\int_0^{\pi}e^{a(\tau)}d\tau + e^{\frac{\gamma\pi}{2}}\int_0^{\theta}e^{a(\tau)}d\tau\right)\right]e^{-a(\theta)-\frac{\gamma\pi}{2}}$$

$$= \frac{1}{Z}\left[1+\frac{e^{\gamma\pi}-1}{\int_0^{2\pi}e^{a(\tau)}d\tau}\int_0^{\pi}e^{a(\tau)}d\tau\right]e^{-a(\theta)-\frac{\gamma\pi}{2}} + \frac{1}{Z}\frac{e^{\gamma\pi}-1}{\int_0^{2\pi}e^{a(\tau)}d\tau}\int_0^{\theta}e^{a(\tau)}d\tau e^{-a(\theta)}$$

$$= \frac{1}{Z}[1+b(\pi)]e^{-\frac{\gamma\pi}{2}}e^{-a(\theta)} + \frac{1}{Z}b(\theta)e^{-a(\theta)}$$

$$= \frac{1}{Z}[1+b(\pi)]e^{-\frac{\gamma\pi}{2}}e^{-a(\theta)} + \psi(\theta) - \frac{1}{Z}e^{-a(\theta)}.$$

If we want to prove $\psi(\theta+\pi)=\psi(\theta)$, we have to verify

$$[1+b(\pi)]e^{-\frac{\gamma\pi}{2}} = 1. \tag{2.15}$$

That is, by using (1.8) again,

$$(e^{\gamma\pi}-1)\int_0^{\pi}e^{a(\tau)}d\tau = (e^{\gamma\pi/2}-1)\int_0^{2\pi}e^{a(\tau)}d\tau. \tag{2.16}$$

In fact, from (1.7) we know that $a(\pi+\theta)=a(\theta)+\frac{\gamma\pi}{2}$. Thus

$$\int_0^{2\pi}e^{a(\tau)}d\tau = \left(\int_0^{\pi}+\int_{\pi}^{2\pi}\right)e^{a(\tau)}d\tau$$

$$= \int_0^{\pi}e^{a(\tau)}d\tau + \int_0^{\pi}e^{a(\pi+\tau)}d\tau$$

$$= (1+e^{\gamma\pi/2})\int_0^{\pi}e^{a(\tau)}d\tau.$$

Multiplying by $(e^{\gamma\pi/2}-1)$ implies (2.16) and completes the proof. □

From this assertion, we know that the rods are symmetric, i.e they have orientations but no directions. This is similar to the result in [16, 17].

In the following we will determine the critical points of α and γ numerically. Set

$$B(\alpha,\eta,\gamma,\theta_0) = \frac{\int_0^{2\pi}\cos 2(\theta-\theta_0)[1+b(\theta)]\ e^{-a(\theta)}d\theta}{\int_0^{2\pi}[1+b(\theta)]\ e^{-a(\theta)}d\theta} + \frac{2\eta}{\alpha} + \frac{\gamma}{2\alpha}\sin 2\theta_0, \tag{2.17}$$

$$F(\alpha,\eta,\gamma,\theta_0) = \frac{\int_0^{2\pi}\sin 2(\theta-\theta_0)[1+b(\theta)]\ e^{-a(\theta)}d\theta}{\int_0^{2\pi}[1+b(\theta)]\ e^{-a(\theta)}d\theta} + \frac{\gamma}{2\alpha}\cos 2\theta_0, \tag{2.18}$$

for the terms obtained in (1.10) and (1.11). We will directly calculate (2.17) and (2.18) for given $\alpha,\gamma,\eta,\theta_0$. Then we take the contour line of value 0 for B and F. The intersection points are what we want to find. The following figures are the contour lines of value 0 of B (continuous line) and F (dashed line) in (figures 2.1–2.6).

From figures (2.1-2.6), we can see that there are multiple points of the contour lines of value 0 of B and F of (2.17) and (2.18), respectively. In the following we give
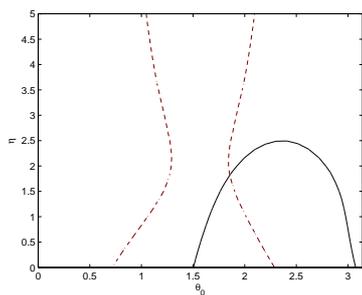
FIG. 2.1. $\alpha = 5.0$ and $\gamma = 3.0$
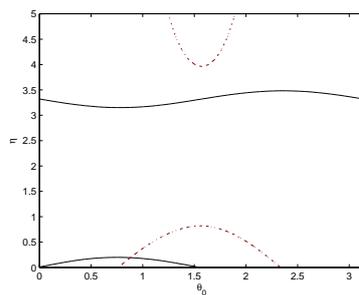
FIG. 2.2. $\alpha = 8.0$ and $\gamma = 0.5$
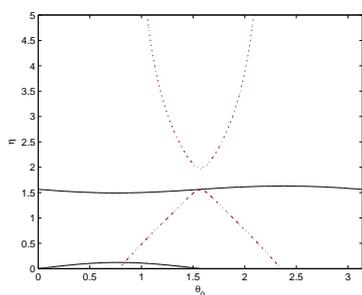
FIG. 2.3. $\alpha = 5.1175$ and $\gamma = 0.1$
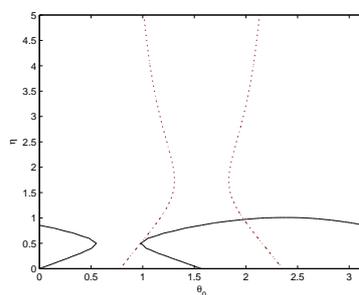
FIG. 2.4. $\alpha = 4.3615$ and $\gamma = 0.1$
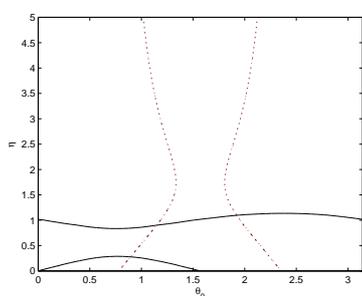
FIG. 2.5. $\alpha = 4.5$ and $\gamma = 0.1$
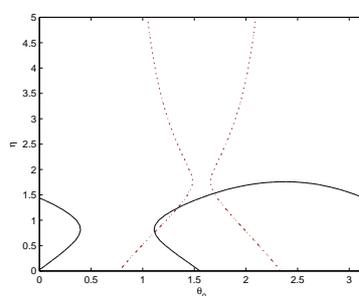
FIG. 2.6. $\alpha = 5.0$ and $\gamma = 0.5$

γ	0.01	0.01	0.01	0.15	0.15	0.15	0.17	0.17	0.2	0.3
η	0.133	0.97	1.06	0.47	0.78	1.12	0.60	1.13	1.15	1.19
θ_0	0.84	1.73	1.94	0.97	1.10	1.91	1.03	1.91	1.90	1.90
En	-0.70	-0.72	-0.72	-0.59	-0.59	-0.63	-0.57	-0.62	-0.60	-0.53

TABLE 2.1. $\alpha = 4.5$, En=energy
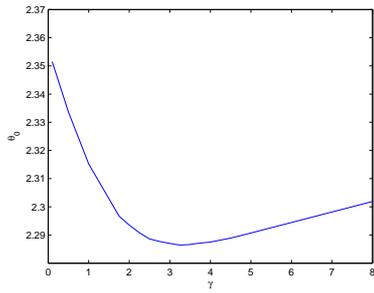
FIG. 2.7. $\alpha = 1.0$
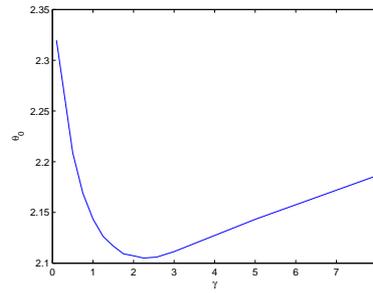
FIG. 2.8. $\alpha = 3.0$
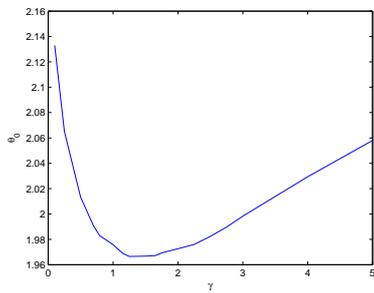
FIG. 2.9. $\alpha = 4.0$
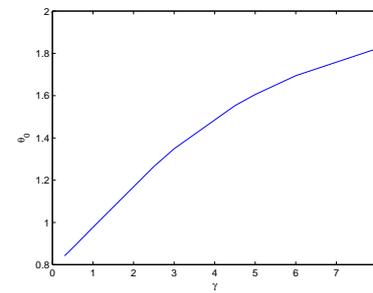
FIG. 2.10. $\alpha = 8.0$

γ	0.4	0.5	0.75	1.0	1.5	2.0	3.0	4.0	4.5	5.0
η	1.23	1.27	1.33	1.38	1.47	1.59	1.73	1.93	2.02	2.03
θ_0	1.88	1.87	1.86	1.86	1.87	1.89	1.93	1.98	1.99	2.06

TABLE 2.2. $\alpha = 4.5$

γ	0.05	0.05	0.05	0.1	0.1	0.1	0.4	0.4	0.4
η	0.07	1.46	1.48	0.14	1.45	1.49	0.57	1.33	1.52
θ_0	0.81	1.44	1.70	0.84	1.43	1.70	1.03	1.38	1.69
$energy$	-0.55	-0.59	-0.60	-0.51	-0.55	-0.56	-0.25	-0.28	-0.34

TABLE 2.3. $\alpha = 5.0$

γ	0.5	0.5	0.5	0.57	0.6	0.8	1.0	1.5	2.0
η	0.77	1.23	1.53	1.54	1.54	1.56	1.57	1.62	1.68
θ_0	1.12	1.34	1.70	1.70	1.70	1.71	1.73	1.75	1.79
$energy$	-0.16	-0.18	-0.27	-0.22	-0.19	-0.14	-0.11	0.48	0.86

TABLE 2.4. $\alpha = 5.0$

γ	2.5	3.0	3.5	4.0	4.5	5.0	6.0	7.0	8.0	10.0
η	1.75	1.82	1.92	2.00	2.10	2.21	2.42	2.64	2.86	3.32
θ_0	1.75	1.86	1.89	1.91	1.94	1.96	2.00	2.03	2.06	2.10

TABLE 2.5. $\alpha=5.0$

γ	0.3	0.5	1.0	3.0	5.0	8.0	10.0	12.0	15.0
η	0.12	0.19	0.38	1.08	1.80	2.85	3.44	3.99	4.76
θ_0	0.84	0.88	0.98	1.35	1.61	1.82	1.91	1.97	2.03

TABLE 2.6. $\alpha=8.0$

γ	0.5	0.8	1.0	3.0	5.0	8.0	10.0	12.0	15.0
η	0.14	0.22	0.28	0.81	1.39	2.38	3.06	3.71	4.63
θ_0	0.86	0.90	0.930	1.23	1.47	1.70	1.79	1.86	1.94

TABLE 2.7. $\alpha=10.0$.

some tables, which are zeros of B and F for different α and γ. These tables show the following facts:

(a) When $0<\alpha<\alpha_1(\alpha_1\approx4.083)$, there is only one pair of (η,θ_0) such that $B=0$ and $F=0$ (figure 2.1). Moreover, for $\alpha\in]0,\alpha_1[$ fixed, the solution (η,θ_0) depends on the shear rate γ and θ_0 is not a monotone function of γ. There is a critical point of γ such that θ_0 attains the minimum. For example, $\gamma=3.5$ is the critical point for $\alpha=1.0$ (figure 2.7). The values $\gamma=2.5,1.5$ are also the critical points for $\alpha=3.0,4.0$ (figures 2.8, 2.9), respectively, while the solution η is an increasing function of γ for α fixed. In fact from the form (2.6) of $a(\theta)$ there is another pair of zeros, denoted by (η^*,θ_0^*), then $\eta^*=-\eta$ and $\theta_0^*=\theta_0+\pi/2$.

(b) When $\alpha_1<\alpha<\alpha_2(\alpha_2\approx5.125)$, there are multiple pairs of solutions (η,θ_0) such that $B=0$ and $F=0$ (ref. Tables 2.1–2.4). The number of solutions depends on the choice of γ. For example, we can see that $(\eta,\theta_0)=(0.1333,0.8374)$, $(0.967,1.728)$, $(1.0596,1.935)$ are solutions of $B=0$ and $F=0$ for $\gamma=0.01$ and $\alpha=4.5$ from Table 2.2. When $\alpha=4.5$ and $\gamma=0.1685$, there are two solutions $(\eta,\theta_0)=(0.6,1.025)$, $(1.1346,1.9092)$. But when $\alpha=4.5$ and $\gamma>0.6$, there is only one solution. Moreover, comparing Table 2.4 and Table 2.2, we can see that γ depends on $\alpha\in]\alpha_1,\alpha_2[$, for which the equations $B=0$ and $F=0$ has multiple solutions. But not all these solutions are stable. In section 4 we will investigate the stability of these solutions.

(c) When $\alpha>\alpha_2$, there is only a pair of solution (η,θ_0) which satisfies $B=0$ and $F=0$ (figure 2.2). Moreover, for $\alpha\in]\alpha_2,\infty[$ fixed, θ_0 and η are increasing functions of the shear rate γ, e.g., from (figure 2.10) we can see the profile of $\theta_0(\gamma)$ for $\alpha=8.0$.

3. Stability of multiple solutions

In this section we will investigate the stability of the multiple solutions with respect to the energy functional. We use (1.6) and (2.11) to obtain

$$E(\psi) = \int_0^{2\pi} [\psi \ln \psi + \frac{1}{2} \psi a(\theta)] d\theta$$

$$= \int_0^{2\pi} \psi[\ln(1 + b(\theta)) - a(\theta) - \ln Z] + \frac{1}{2}\psi \left[\frac{\alpha}{2} + \eta \cos 2(\theta - \theta_0) + \frac{\gamma\theta}{2}\right] d\theta.$$

Then (2.6) gives

$$E(\psi) = \int_0^{2\pi} \left\{ \psi \left[\ln(1 + b(\theta)) - \left(\frac{\alpha}{2} + \eta \cos 2(\theta - \theta_0) + \frac{\gamma\theta}{2} \right) - \ln Z \right] \right.$$

$$\left. + \frac{1}{2}\psi \left[\frac{\alpha}{2} + \eta \cos 2(\theta - \theta_0) + \frac{\gamma\theta}{2} \right] \right\} d\theta$$

$$= \int_0^{2\pi} \psi \left\{ \ln(1 + b(\theta)) - \frac{1}{2}\left[\frac{\alpha}{2} + \eta \cos 2(\theta - \theta_0) + \gamma\theta - \frac{\gamma}{4}\sin 2\theta \right] - \ln Z \right\} d\theta$$

$$= \frac{1}{Z}\int_0^{2\pi} [1 + b(\theta)]e^{-a(\theta)} \left[\ln(1 + b(\theta)) - \frac{\eta}{2}\cos 2(\theta - \theta_0) - \frac{\gamma\theta}{4} \right] d\theta$$

$$- \frac{\alpha}{4} - \ln Z.$$

Thus, we can calculate the energy functional for η, θ_0 determined by (1.10) and (1.11) as α, γ given. For example, from Table 2.1, we can see that the energies of points $(\eta, \theta_0) = (0.967, 1.728), (1.0596, 1.935)$ are almost -0.72 and less than the energy of other solution as $\alpha = 4.5$ and $\gamma = 0.01$. So these two points are stable points. Here we show the Table 2.3 and 2.4 to display the energy for the multiple solutions of (1.10) and (1.11) for $\alpha = 4.5, 5.0$, respectively, and γ given. The points with low values are the stable points.

4. Conclusion

In this work we have given the explicit expression of the equilibrium to the 1D Doi model in the shear flow. The difference from this expression to the Maxwell-Boltzmann distribution without flow can be seen. Here are two parameters, the interaction intensity among particles α and the shear rate γ, to determine the states of the particles in the general one dimension shear flow of polymeric fluids. According to our discussion, we know that the equilibrium of these particles depends on the competition between α and γ. When the interaction intensity α is less than the first critical point $\alpha_1 \approx 4.083$ or larger than the second critical point $\alpha_2 \approx 5.125$, the steady state of these molecules is uniquely determined by α and γ, where γ can be arbitrary. But when $\alpha \in]\alpha_1, \alpha_2[$, it is another story. There are multiple steady states of these particles. It is possible to have one, two, or three equilibria. This is completely dependent on the shear rate. When the shear rate is very large, the equilibrium is also uniquely determined. While the shear rate is not large enough, the equilibrium will be multiple steady states. However, not all equilibria are stable. From the discussion of the energy functional, we can see that it is possible that there are one or two stable equilibria for some α and γ.

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